Pergamon

Computers Math. Applic. Vol. 30, No. 2, pp. 17–25, 1995

0898-1221/95 $9.50 + 0.00

0898-1221(95)00074-7

Least Squares Methods for Optimal Shape Design Problems

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(Received December 1994; accepted January 1995)

Abstract—A Least-Squares method for solving an optimal shape design problem which appears in semiconductor device physics is described. Discretization by finite element methods is used for numerical solving. An example and experimental results are presented.

Keywords—Least squares, Finite element, Optimal shape design, Free boundary problem, Semiconductor problem.

1. INTRODUCTION

Free boundary problems appear in modeling a wide variety of physical phenomena [1–6]. They have been studied extensively by means of variational inequalities approximated by finite differences or finite element methods [7–9]. The use of least-squares finite element methods for solving elliptic problems presents a series of advantages over the Galerkin methods: it gives better order approximations under appropriate regularity hypotheses [10], the algebraic system formed by approximation is symmetric and positive definite [10], and inhomogeneous boundary conditions can be treated as part of the least-squares functional [11]. Here we shall consider least-squares formulations for free boundary problems. The major attraction of this approach is that the free boundary is a part of the functional that is to be minimized. Numerical results presented in this paper show that this gives approximations which quadratically converge to the exact free boundary. To illustrate the basic approach, we shall use as a model a bilateral optimal shape design problem which appears in semiconductor device physics [12] and has been approached numerically in [13] by a Galerkin method. One of the primary reasons for this choice is that in applications the accurate approximation of the free boundary is the item of primary physical interest, and our numerical results indicate that a least-squares formulation is well suited to the type of context.

2. THE MODEL PROBLEM

Consider the bilateral free boundary problem:
Find $\alpha, \beta \in C^1[0,1]$ *and* $u \in C(\overline{\Omega}) \cap H^1(\Omega)$ *such that:*

$$-\Delta u = f, \qquad \text{in } \Omega, \tag{1}$$

$$u = g_1, \qquad \text{on } \Gamma_1, \tag{2}$$

$$u = g_2, \qquad \text{on } \Gamma_2, \tag{3}$$

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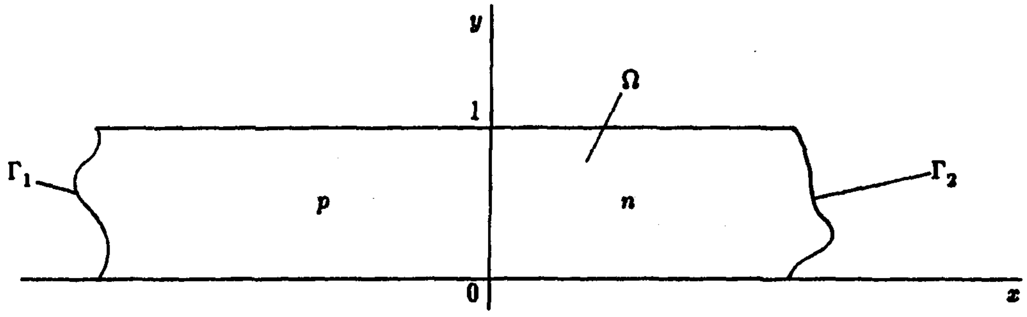


Figure 1. The domain Ω for the model problem.

$$\frac{\partial u}{\partial \nu} = 0, \qquad \text{on } \Gamma = \partial\Omega, \tag{4}$$

$$C_1 \le -\beta(y) \le C_2 < C_3 \le \alpha(y) \le C_4, \qquad \text{all } y \in [0,1],$$

where $\Omega \subset \mathbb{R}^2, C_1$–$C_4$ *are constants,* f *is bounded on* $\widehat{\Omega} = [C_1, C_4] \times [0,1]$ *and is such that* $\int_\Omega f = 0$, g_1 *and* g_2 *are given functions on* Γ_1 *and* Γ_2*, respectively, and*

$$\begin{aligned}
&\Omega = \Omega(\alpha,\beta) = \left\{(x,y) \in \mathbb{R}^2 : 0 \le y \le 1, -\beta(y) \le x \le \alpha(y) \text{ all } y \in [0,1]\right\},\\
&\Gamma = \Gamma(\alpha,\beta) = \partial\,\Omega,\\
&\Gamma_1 = \Gamma_1(\beta) = \left\{(x,y) \in \mathbb{R}^2 : x = -\beta(y), 0 \le y \le 1\right\} \subset \Gamma(\alpha,\beta),\\
&\Gamma_2 = \Gamma_2(\alpha) = \left\{(x,y) \in \mathbb{R}^2 : x = \alpha(y), 0 \le y \le 1\right\} \subset \Gamma(\alpha,\beta).
\end{aligned}$$

The problem has been studied in [13] by means of variational inequalities.

Notice that an equivalent formulation is (see [10]):

$$\nabla u - \lambda = 0, \qquad \text{in } \Omega, \tag{5}$$

$$\operatorname{div} \lambda + f = 0, \qquad \text{in } \Omega, \tag{6}$$

$$u = g_1, \qquad \text{on } \Gamma_1, \tag{7}$$

$$u = g_2, \qquad \text{on } \Gamma_2, \tag{8}$$

$$\lambda \cdot \nu = 0, \qquad \text{on } \Gamma. \tag{9}$$

3. LEAST-SQUARES FORMULATION AND APPROXIMATION

Like in [13], assume that $(\alpha,\beta) \in U_{ad}$, where

$$\begin{aligned}
U_{ad} = \Bigg\{ &(\alpha,\beta) : \alpha,\beta \in C^1[0,1], C_1 \le -\beta(y) \le C_2 < C_3 \le \alpha(y) \le C_4 \text{ all } y \in [0,1],\\
&|\alpha(y) - \alpha(\overline{y})| \le C_5|y - \overline{y}| \text{ all } y,\overline{y} \in [0,1],\\
&|\beta(y) - \beta(\overline{y})| \le C_6|y - \overline{y}| \text{ all } y,\overline{y} \in [0,1], \int_{\Omega(\alpha,\beta)} f = 0 \Bigg\}
\end{aligned} \tag{10}$$

is the set of admissible controls, with C_1–C_6 are constants, chosen such that $U_{ad} \neq \emptyset$. Let $\mathcal{O} = \{\Omega(\alpha,\beta) : \alpha \in U_{ad}\}$. For $\Omega = \Omega(\alpha,\beta) \in U_{ad}$, we define the following functional:

$$\begin{aligned}
\Phi(v,\psi,\alpha,\beta) = w_0 \int_\Omega (\nabla v - \psi)^2 + w_1 \int_\Omega (\operatorname{div} \psi + f)^2&\\
+ w_2 \left(\int_{\Gamma_1} (v - g_1)^2 + \int_{\Gamma_2} (v - g_2)^2 \right) + w_3 \int_\Gamma (\psi \cdot \nu)^2&
\end{aligned} \tag{11}$$

where w_0, w_1, w_2 and w_3 are weights to be specified later. Let $\mathcal{V}(\alpha,\beta) = H^1(\Omega(\alpha,\beta)), \mathcal{S}(\alpha,\beta) = H^1(\Omega(\alpha,\beta))$. A Least-Squares formulation of the problem (5–9) is:

$$\text{Min } \Phi(v,\psi,\alpha,\beta) \tag{12}$$

where the minimum is taken over all $v \in \mathcal{V}(\alpha,\beta), \psi \in \mathcal{S}(\alpha,\beta)$ *and* $(\alpha,\beta) \in U_{ad}$.

In order to obtain a discretization, we introduce finite dimensional spaces $\mathcal{V}_h$ and $\mathcal{S}_\delta$, where $h, \delta > 0$ are discretization parameters. Then an approximate problem associated with (12) is:

$$\text{Min } \Phi_{h,\delta}\left(v^h, \psi^\delta, \alpha_{h,\delta}, \beta_{h,\delta}\right) \tag{13}$$

where the minimum is taken over all $v^h \in \mathcal{V}_h, \psi^\delta \in \mathcal{S}_\delta$ *and* $(\alpha_{h,\delta}, \beta_{h,\delta}) \in U_{ad}^{h,\delta}, \Phi_{h,\delta}$ *is a discretization of* Φ, *and* $U_{ad}^{h,\delta}$ *is a discretization of* U_{ad}.

To be more specific for the model problem (5–9), let $0 = y_0 < y_1 < \cdots < y_{N(h)} = 1$ be a partition of $[0,1]$, such that $\max_{1\le j\le N(h)} |y_j - y_{j-1}| \le h$ (see [13]). Assume that $h = \delta$ and $\mathcal{S}_\delta = \mathcal{V}_h \times \mathcal{V}_h$, and let U_{ad}^h be the set of admissible approximating controls, defined by:

$$U_{ad}^h = \left\{ \begin{aligned} &(\alpha_h,\beta_h) : \alpha_h, \beta_h \in C^0[0,1], \alpha_h, \beta_h \text{ are piecewise polynomials of degree } k, \\ &C_1 \le -\beta_h(y) \le C_2 < C_3 \le \alpha_h(y) \le C_4 \text{ all } y \in [0,1], \int_{\Omega(\alpha_h,\beta_h)} f = 0 \\ &|\alpha_j - \alpha_{j-1}| \le C_5|y_j - y_{j-1}|, |\beta_j - \beta_{j-1}| \le C_6|y_j - y_{j-1}|, j = 1,\ldots,N(h) \end{aligned} \right\} \tag{14}$$

where C_1–C_6 are constants chosen such that $U_{ad}^h \ne \emptyset$, and $\alpha_j = \alpha_h(y_j)$, $\beta_j = \beta_h(y_j)$, $j = 1,\ldots,N(h)$ (see Figure 2).

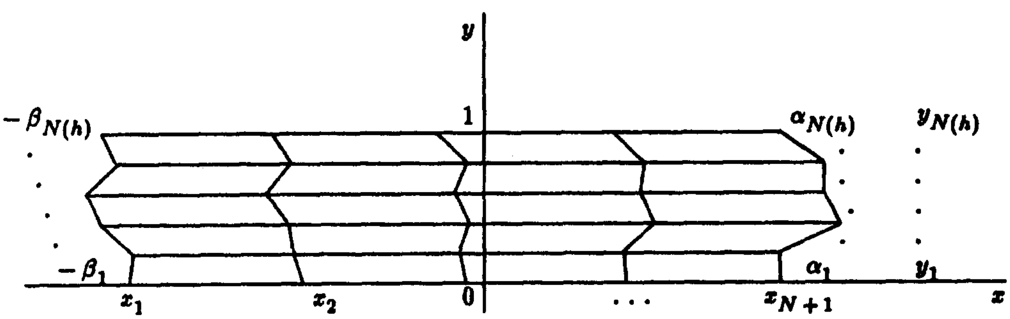


Figure 2. The discretized domain Ω_h.

Let $\mathcal{O}_h = \{\Omega(\alpha_h,\beta_h) : (\alpha_h,\beta_h) \in U_{ad}^h\}$. Let k be chosen such that $\mathcal{O}_h \subset \mathcal{O}$ (see comments on the grid in [13]). Let $g_{1,h}$ and $g_{2,h}$ be approximants of g_1 and g_2 over $\Gamma_1(\beta_h)$ and $\Gamma_2(\alpha_h)$, respectively (they can be interpolates or appropriate projections of g_1 and g_2 onto $\Gamma_1(\beta_h)$ and $\Gamma_2(\alpha_h)$). Now assume $\mathcal{V}_h \subset H^1(\Omega(\alpha_h,\beta_h))$ is a finite dimensional subspace. Denote $\Omega_h = \Omega(\alpha_h,\beta_h), \Gamma_h = \Gamma(\alpha_h,\beta_h), \Gamma_{1,h} = \Gamma_1(\beta_h), \Gamma_{2,h} = \Gamma_2(\alpha_h)$.

Let

$$\begin{aligned} \Phi_h\left(v^h,\psi^h,\alpha_h,\beta_h\right) &= w_0(h)\int_{\Omega_h}\left(\nabla v^h - \psi^h\right)^2 + w_1(h)\int_{\Omega_h}\left(\operatorname{div}\psi^h + f\right)^2 \\ &+ w_2(h)\left(\int_{\Gamma_{1,h}}\left(v^h - g_{1,h}\right)^2 + \int_{\Gamma_{2,h}}\left(v^h - g_{2,h}\right)^2\right) + w_3(h)\int_{\Gamma_h}\left(\psi^h\cdot\nu_h\right)^2 \end{aligned} \tag{15}$$

where ν_h denotes the normal to Γ_h. Now (13) becomes:

$$\text{Min } \Phi_h\left(v^h, \psi^h, \alpha_h, \beta_h\right) \tag{16}$$

where the minimum is taken over all $v^h \in \mathcal{V}_h, \psi^h \in \mathcal{V}_h \times \mathcal{V}_h$ *and* $(\alpha_h, \beta_h) \in U^h_{ad}$.

This leads to solving the following system of equations for $u_h, \lambda_h, \boldsymbol{\alpha} = [\alpha_1, \dots \alpha_{N(h)}]^\top$ and $\boldsymbol{\beta} = [\beta_1, \dots \beta_{N(h)}]^\top$:

$$w_0(h) \int_{\Omega_h} (\nabla u_h - \lambda_h)\nabla v^h + w_2(h)\left(\int_{\Gamma_{1,h}} (u_h - g_{1,h})v^h + \int_{\Gamma_{2,h}} (u_h - g_{2,h})v^h\right) = 0, \quad \text{all } v^h \in \mathcal{V}_h, \tag{17}$$

$$- w_0(h) \int_{\Omega_h} (\nabla u_h - \lambda_h)\psi^h + w_1(h) \int_{\Omega_h} (\text{div } \lambda_h + f)\text{div } \psi^h + w_3(h) \int_{\Gamma_h} (\lambda_h \cdot \nu_h)(\psi^h \cdot \nu_h) = 0, \quad \text{all } \psi^h \in \mathcal{V}_h, \tag{18}$$

$$\frac{\partial \Phi_h}{\partial \alpha_j} = 0, \qquad \text{all } j = 1, \dots, N(h), \tag{19}$$

$$\frac{\partial \Phi_h}{\partial \beta_j} = 0, \qquad \text{all } j = 1, \dots, N(h). \tag{20}$$

NOTE. Assuming that the grid is uniform in the y-direction, with $N(h) = M$ and meshspacing $h_y = 1/M$, the discretization parameter h in the x-direction is actually an M-dimensional vector $[h_1, \dots, h_M]^\top$, with $h_j = h_j(\alpha_j, \beta_j), j = 1, \dots, M$; i.e., h_j represents the discretization parameter at the j^{th} level (see Figure 2). For example, if one chooses to associate with Ω_h a mesh which is uniform in the x-direction and has the same number of nodes $N+1$ at each level j, then $h_j = (\alpha_j + \beta_j)/N, j = 1, \dots, M$. A particular case will be presented in Section 4.

4. EXAMPLE

Assume that $g_1(x, y) = c_1$, all $(x, y) \in \Gamma_1$ (g_1 is constant), $g_2(x, y) = c_2$, all $(x, y) \in \Gamma_2$ (g_2 is constant) and $f(x, y) = f(x)$, all $y \in [0, 1]$. Then α, β and u are also expected to depend only on x, and the problem can be reduced to a one-dimensional one (also see the example in [13]):

Find $\alpha, \beta \in \mathbb{R}$ *and* u *on* $[-\beta, \alpha]$ *such that:*

$$-\frac{d^2u}{dx^2} = f, \qquad \text{on } (-\beta, \alpha), \qquad \text{where } f \text{ is such that } \int_{-\beta}^{\alpha} f = 0, \tag{21}$$

$$u(-\beta) = c_1, \qquad (c_1 \text{ given}) \tag{22}$$

$$u(\alpha) = c_2, \qquad (c_2 \text{ given}) \tag{23}$$

$$\frac{du}{dx}(-\beta) = \frac{du}{dx}(\alpha) = 0, \tag{24}$$

or:

$$-\frac{d\lambda}{dx} = f, \qquad \text{on } (-\beta, \alpha), \tag{25}$$

$$\frac{du}{dx} - \lambda = 0, \qquad \text{on } (-\beta, \alpha), \tag{26}$$

$$u(-\beta) = c_1, \tag{27}$$

$$u(\alpha) = c_2, \tag{28}$$

$$\lambda(-\beta) = \lambda(\alpha) = 0. \tag{29}$$

The Least-Squares functional is:

$$\Phi(v,\psi,\alpha,\beta)=w_0\int\limits_{-\beta}^{\alpha}\left(\frac{dv}{dx}-\psi\right)^2+w_1\int\limits_{-\beta}^{\alpha}\left(\frac{d\psi}{dx}+f\right)^2$$
$$+w_2\left((v(-\beta)-c_1)^2+(v(\alpha)-c_2)^2\right)+w_3\left(\psi(-\beta)^2+\psi(\alpha)^2\right), \quad (30)$$

and we have to minimize $\Phi(v,\psi,\alpha,\beta)$ over all $v\in\mathcal{V},\psi\in\mathcal{S}$ and $(\alpha,\beta)\in U_{ad}$, where $\mathcal{V}=\mathcal{S}=H^1(-\beta,\alpha)$ and

$$U_{ad}=\left\{(\alpha,\beta)\in\mathbb{R}^2: C_1\le-\beta\le C_2<C_3\le\alpha,\int\limits_{-\beta}^{\alpha}f=0\right\}. \quad (31)$$

If we introduce finite dimensional subspaces $\mathcal{V}_h\subset\mathcal{V}$ and $\mathcal{S}_\delta\subset\mathcal{S}$, the approximate problem associated with (25–29) is:

$$\text{Min }\Phi\left(v^h,\psi^\delta,\alpha,\beta\right) \quad (32)$$

where the minimum is taken over all $v^h\in\mathcal{V}_h,\psi^\delta\in\mathcal{S}_\delta$ *and* $(\alpha,\beta)\in U_{ad}$.

This leads to the following algebraic system:

Find $u_h\in\mathcal{V}_h$, $\lambda_\delta\in\mathcal{S}_\delta$ *and* $(\alpha,\beta)\in U_{ad}$ *such that:*

$$w_0\int\limits_{-\beta}^{\alpha}\left(\frac{du_h}{dx}-\lambda_\delta\right)\frac{dv^h}{dx}+w_2\left((u_h(-\beta)-c_1)\,v^h(-\beta)+(u_h(\alpha)-c_2)\,v^h(\alpha)\right)=0,$$
$$\text{all } v^h\in\mathcal{V}_h, \quad (33)$$

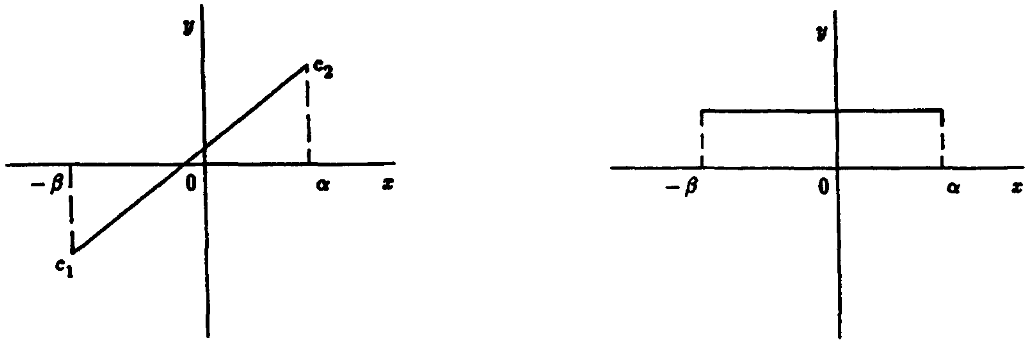
$$-w_0\int\limits_{-\beta}^{\alpha}\left(\frac{du_h}{dx}-\lambda_\delta\right)\psi^\delta+w_1\int\limits_{-\beta}^{\alpha}\left(\frac{d\lambda_\delta}{dx}+f\right)\frac{d\psi^\delta}{dx}$$
$$+w_3\left(\lambda_\delta(-\beta)\psi^\delta(-\beta)+\lambda_\delta(\alpha)\psi^\delta(\alpha)\right)=0, \qquad \text{all } \psi^\delta\in\mathcal{S}_\delta, \quad (34)$$

$$\frac{\partial\Phi_h}{\partial\alpha}=0, \quad (35)$$
$$\frac{\partial\Phi_h}{\partial\beta}=0. \quad (36)$$

To fix the ideas, assume that a uniform mesh $-\beta=x_1<x_2<\cdots<x_{N+1}=\alpha$ is associated with $[-\beta,\alpha]$, of meshspacing $h=h(\alpha,\beta)=(\alpha+\beta)/N$; also assume that $\mathcal{S}_\delta=\mathcal{V}_h=\text{span }[\phi_1,\ldots,\phi_{N+1}]$, where each ϕ_j is a linear function having the value 1 at the j^{th} node and 0 in rest. Then, in (33–36), we look for u_h and λ_h of the form: $u_h=\sum_{j=1}^{N+1}u_j\phi_j$ and $\lambda_h=\sum_{j=1}^{N+1}\lambda_j\phi_j$; also, the midpoint rule can be used for integration and the system (33–36) is:

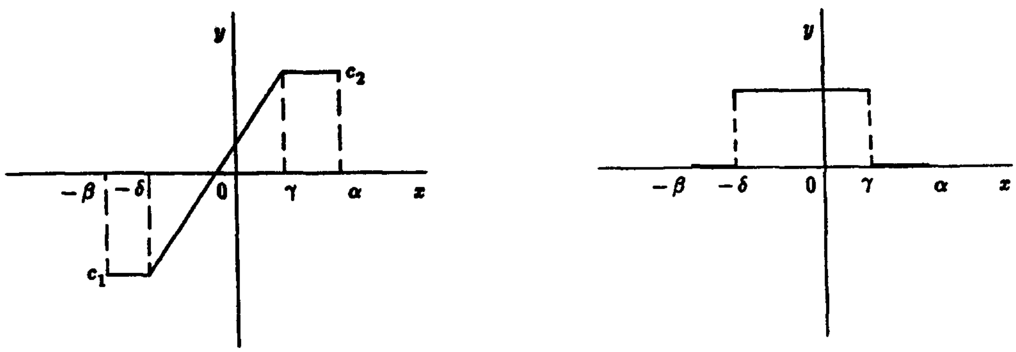
Find $\boldsymbol{u}=[u_1,\ldots,u_{N+1}]^\top\in\mathbb{R}^{N+1},\boldsymbol{\lambda}=[\lambda_1,\ldots,\lambda_{N+1}]^\top\in\mathbb{R}^{N+1}$ *and* $(\alpha,\beta)\in U_{ad}$ *such that:*

$$\frac{w_0}{h}(u_1-u_2)+\frac{w_0}{2}(\lambda_1+\lambda_2)+w_2(u_1-c_1)=0, \quad (37)$$
$$\frac{w_0}{h}(-u_{j-1}+2u_j-u_{j+1})+\frac{w_0}{2}(-\lambda_{j-1}+\lambda_{j+1})=0, \qquad j=2,\ldots,N, \quad (38)$$
$$\frac{w_0}{h}(-u_N+u_{N+1})+\frac{w_0}{2}(-\lambda_N-\lambda_{N+1})+w_2(u_{N+1}-c_2)=0, \quad (39)$$



(a) Initial guess for $u_h^{(0)}$. (b) Initial guess for $\lambda_h^{(0)}$.

Figure 3.



(a) Initial guess for $u_h^{(0)}$. (b) Initial guess for $\lambda_h^{(0)}$.

Figure 4.

$$\frac{w_0}{2}(u_1 - u_2) + \left(\frac{w_0 h}{3} + \frac{w_1}{h}\right)\lambda_1 + \left(\frac{w_0 h}{6} - \frac{w_1}{h}\right)\lambda_2 - w_1 f\left(\frac{x_1 + x_2}{2}\right) + w_3\lambda_1 = 0, \tag{40}$$

$$\frac{w_0}{2}(u_{j-1} - u_{j+1}) + \left(\frac{w_0 h}{6} - \frac{w_1}{h}\right)\lambda_{j-1} + 2\left(\frac{w_0 h}{3} + \frac{w_1}{h}\right)\lambda_j + \left(\frac{w_0 h}{6} - \frac{w_1}{h}\right)\lambda_{j+1} + w_1\left(f\left(\frac{x_{j-1} + x_j}{2}\right) - f\left(\frac{x_j + x_{j+1}}{2}\right)\right) = 0, \qquad j = 2, \dots, N, \tag{41}$$

$$\frac{w_0}{2}(u_N - u_{N+1}) + \left(\frac{w_0 h}{6} - \frac{w_1}{h}\right)\lambda_N + \left(\frac{w_0 h}{3} + \frac{w_1}{h}\right)\lambda_{N+1} + w_1 f\left(\frac{x_N + x_{N+1}}{2}\right) + w_3\lambda_{N+1} = 0, \tag{42}$$

$$\frac{\partial \Phi_h}{\partial \alpha} = 0, \tag{43}$$

$$\frac{\partial \Phi_h}{\partial \beta} = 0. \tag{44}$$

If the weights w_0, w_1, w_2 and w_3 depend on h, then:

$$\frac{\partial \Phi}{\partial \alpha} = \frac{w_0'}{N}\int_{-\beta}^{\alpha}\left(\frac{du}{dx} - \lambda\right)^2 + w_0\left(\frac{du}{dx} - \lambda\right)^2\bigg|_{x=\alpha} + \frac{w_1'}{N}\int_{-\beta}^{\alpha}\left(\frac{d\lambda}{dx} + f\right)^2$$

$$
\begin{aligned}
&+ w_1 \left(\frac{d\lambda}{dx} + f\right)^2\bigg|_{x=\alpha} + \frac{w_2'}{N}\left((u(-\beta) - c_1)^2 + (u(\alpha) - c_2)^2\right) \\
&+ 2w_2\,(u(\alpha) - c_2)\,u'(\alpha) + \frac{w_3'}{N}\left(\lambda(-\beta)^2 + \lambda(\alpha)^2\right) + 2w_3\lambda(\alpha)\lambda'(\alpha),
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial\Phi}{\partial\beta} = \frac{w_0'}{N}\int_{-\beta}^{\alpha}\left(\frac{du}{dx} - \lambda\right)^2 &+ w_0\left(\frac{du}{dx} - \lambda\right)^2\bigg|_{x=-\beta} + \frac{w_1'}{N}\int_{-\beta}^{\alpha}\left(\frac{d\lambda}{dx} + f\right)^2 \\
&+ w_1\left(\frac{d\lambda}{dx} + f\right)^2\bigg|_{x=-\beta} + \frac{w_2'}{N}\left((u(-\beta) - c_1)^2 + (u(\alpha) - c_2)^2\right) \\
&- 2w_2\,(u(-\beta) - c_1)\,u'(-\beta) + \frac{w_3'}{N}\left(\lambda(-\beta)^2 + \lambda(\alpha)^2\right) - 2w_3\lambda(-\beta)\lambda'(-\beta).
\end{aligned}
$$

We need to obtain u and λ so that $u'(\alpha) = \lambda(\alpha)$ and $u'(-\beta) = \lambda(-\beta)$, and also: $\lambda'(\alpha) = -f(\alpha)$, $\lambda'(-\beta) = -f(-\beta)$, so impose:

$$
\left(\frac{du}{dx} - \lambda\right)^2\bigg|_{x=\alpha} = \left(\frac{du}{dx} - \lambda\right)^2\bigg|_{x=-\beta} = \left(\frac{d\lambda}{dx} + f\right)^2\bigg|_{x=\alpha} = \left(\frac{d\lambda}{dx} + f\right)^2\bigg|_{x=-\beta} = 0.
$$

Now the equations (43,44) in the system are:

$$
\begin{aligned}
\frac{w_0'}{N}\int_{-\beta}^{\alpha}\left(\frac{du_h}{dx} - \lambda_h\right)^2 + \frac{w_1'}{N}\int_{-\beta}^{\alpha}\left(\frac{d\lambda_h}{dx} + f\right)^2 + \frac{w_2'}{N}\left((u_1 - c_1)^2 + (u_{N+1} - c_2)^2\right) \\
+ 2w_2(u_{N+1} - c_2)\lambda_{N+1} + \frac{w_3'}{N}\left(\lambda_1^2 + \lambda_{N+1}^2\right) - 2w_3\lambda_{N+1}f(\alpha) = 0, \quad (45)
\end{aligned}
$$

$$
\begin{aligned}
\frac{w_0'}{N}\int_{-\beta}^{\alpha}\left(\frac{du_h}{dx} - \lambda_h\right)^2 + \frac{w_1'}{N}\int_{-\beta}^{\alpha}\left(\frac{d\lambda_h}{dx} + f\right)^2 + \frac{w_2'}{N}\left((u_1 - c_1)^2 + (u_{N+1} - c_2)^2\right) \\
- 2w_2(u_1 - c_1)\lambda_1 + \frac{w_3'}{N}\left(\lambda_1^2 + \lambda_{N+1}^2\right) + 2w_3\lambda_1 f(-\beta) = 0. \quad (46)
\end{aligned}
$$

To solve this nonlinear algebraic system, the Newton's method can be used.

Possible choices for w_0, w_1, w_2 and w_3 are:

$$
w_0(h) = w_1(h) = 1, \quad w_2(h) = h^{-1}, \quad w_3(h) = h \tag{47}
$$

or

$$
w_0(h) = w_1(h) = w_2(h) = 1, \quad w_3(h) = h^2. \tag{48}
$$

Like in most applications, we shall use (47) in the calculations described below.

5. EXPERIMENTAL RESULTS

The experimental results we present refer to the example in Section 4, with the given data: $c_1 = -2$, $c_2 = 2$, $f(x) = 6x$, which correspond to the exact solution: $u(x) = x(3 - x^2)$, all $x \in [-1, 1]$. The weights used in the Least-Squares functional were: $w_0 = w_1 = 1$, $w_2 = h^{-1}$, $w_3 = h$. The Newton's algorithm is used to solve the algebraic system, starting from an initial guess $\boldsymbol{u}^{(0)}$, $\boldsymbol{\lambda}^{(0)}$, $\alpha^{(0)}$, $\beta^{(0)}$, where $u_j^{(0)} = u_h^{(0)}(x_j)$ and $\lambda_j^{(0)} = \lambda_h^{(0)}(x_j)$ for $j = 1, \dots, N+1$, and $u_h^{(0)}$, $\lambda_h^{(0)}$ are the functions shown in Figure 3(a)–(b) or those shown in Figure 4(a)–(b). In Figure 3, $u_h^{(0)}$ is linear on $[-\beta, \alpha]$ with given values c_1 and c_2, respectively, at endpoints, and accordingly, $\lambda_h^{(0)}$ is constant on $[-\beta, \alpha]$, $\lambda_h^{(0)} = (c_2 - c_1)/(\alpha + \beta)$. The shapes of the functions

Table 1. The number of Newton iterations for $\epsilon = 10^{-3}$.

Initial $\alpha = \beta$:	Number of Newton iterations		
	$N = 8$	$N = 16$	$N = 32$
.6	14	13	11
.7	14	12	12
.8	13	12	11
.9	12	11	10
1.0	11	10	8
1.1	10	7	4
1.2	9	4	8
1.3	5	9	9
1.4	8	9	10
1.5	9	10	10
1.6	10	10	13

Table 2. The computed α and β; the L^2-error and the H^1-error ($\alpha^{(0)} = \beta^{(0)} = 1.2, \epsilon = 10^{-5}$).

N	Computed α and β	$\left\lVert u - u_h^{(k)} \right\rVert_{L^2}$	$\left\lVert u - u_h^{(k)} \right\rVert_{H^1}$
8	1.007036	.6187(−2)	.2789(−1)
16	1.001736	.1524(−2)	.6920(−2)
32	1.000429	.3753(−3)	.1731(−2)
6	1.012626	.1107(−1)	.5002(−1)
12	1.003110	.2736(−2)	.1231(−1)
24	1.000768	.6732(−3)	.3074(−2)

Table 3. Error rate for α and β, obtained for $\epsilon = 10^{-7}$ in (49).

N	Errors for α and β	Rate
4	.2920(-1)	
		4.15
8	.7029(-2)	
		4.02
16	.1741(-2)	
		4.00
32	.4343(-2)	
6	.1261(-1)	
		4.06
12	.3103(-2)	
		4.01
24	.7725(-3)	

in Figure 4 are suggested by condition (24); i.e., for some γ, δ such that $-\beta < -\delta < C_2$ and $C_3 < \gamma < \alpha$, $u_h^{(0)}$ is continuous, constant with values c_1 and c_2 on $[-\beta, -\delta]$ and $[\gamma, \alpha]$, respectively, and linear in rest, and accordingly, $\lambda_h^{(0)}$ is zero on $[-\beta, -\delta]$ and $[\gamma, \alpha]$ and constant ($\lambda_h^{(0)} = (c_2 - c_1)/(\gamma + \delta)$) in rest.

Newton's iterations are applied until

$$\left|\alpha^{(k)} - \alpha^{(k-1)}\right| + \left|\beta^{(k)} - \beta^{(k-1)}\right| < \epsilon, \tag{49}$$

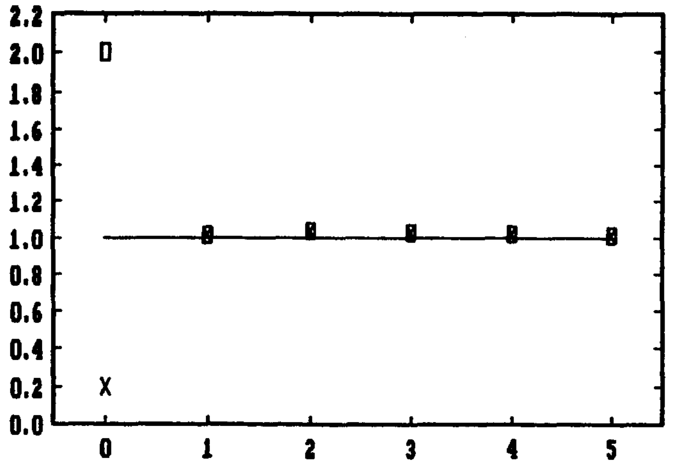


Figure 5. Convergence of α and β (exact: $\alpha = \beta = 1$); $\alpha^{(0)} = 2.0$, $\beta^{(0)} = .2$, $\epsilon = 10^{-3}$, $N = 8$.

and then direct solving (by least-squares) is performed on $[-\beta^{(k)}, \alpha^{(k)}]$. Table 1 shows the number of Newton iterations needed for the stopping criterion to be satisfied, with $\epsilon = 10^{-3}$. Table 2 shows the L^2- and H^1-errors for u, and the computed α and β. Figure 5 shows the convergence of $\alpha^{(k)}$ and $\beta^{(k)}$, from the initial choices $\alpha^{(0)} = 2.0$, $\beta^{(0)} = .2$, for $N = 8$ (exact: $\alpha = \beta = 1$). The errors for α and β listed in Table 3 suggest that $|\alpha^{(k)} - \alpha|$ and $|\beta^{(k)} - \beta|$ are of $O(N^{-2})$ as $k \to \infty$.

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